# On the Calculation of the Parabolic Cylinder Functions. II. The Function $V(a, x)^{*}$ 

In an earlier paper [1], we reported a new procedure for obtaining very accurate values of the parabolic cylinder function $U(a, x)$ over a critical range of the positive $\mathbf{x}$-axis, which involves solving an integral representation by Gaussian quadrature. The method described in [1] is not applicable for negative values of $\mathbf{x}$. The purpose of this note is to report the calculation of the other parabolic cylinder function $V(a, x)$ which is related to $U(a,-x)$ in a simple way.
Our original intention was to obtain $V(a, x)$ in a manner analogous to that used in [1] for $U(a, x)$, that is by finding an integral representation and employing the algorithm described therein to obtain a solution. However, an extensive search of the literature failed to produce such an integral representation for $V(a, x)$. An alternative route is provided by the relationship [2]

$$
\begin{equation*}
\pi V(a, x)=\Gamma[a+(1 / 2)][U(a, x) \sin \pi a+U(a,-x)] . \tag{1}
\end{equation*}
$$

We have used an integral expression for $U(a,-x)$ which combined with the results of [1] for $U(a, x)$ allows accurate values of $V(a, x)$.
An integral equation for $U(a, x)$ applicable for negative values of $\mathbf{x}$ is given by Gradshteyn and Ryzhik [3]

$$
\begin{equation*}
\int_{0}^{\infty} z^{\nu-1} e^{-\beta z^{2}-x z} d z=(2 \beta)^{-\nu / 2} \Gamma(\nu) \exp \left(x^{2} /(8 \beta)\right) D_{-\nu}\left(x /(2 \beta)^{1 / 2}\right) \tag{2}
\end{equation*}
$$

For our purposes, $\beta=\frac{1}{2}$, and in the current notation $U(a, x)=D_{-a-1 / 2}(x)$, so,

$$
\begin{equation*}
U(a, x)=\left[\exp \left(-x^{2} / 4\right) / \Gamma(a+1 / 2)\right] \int_{0}^{\infty} z^{a-1 / 2} e^{-\left(z^{2} / 2\right)-x z} d z \tag{3}
\end{equation*}
$$

subject to the restriction $a>-\frac{1}{2}$ because of the presence of the gamma function.

[^0]The integral in Eq. (3) was solved by Simpson's Rule integration. The truncation error for this method is given by [4]

$$
\begin{equation*}
E_{s}(x)=-\left(z_{2}-z_{1}\right)\left((\Delta z)^{4} / 180\right) f^{(4)}(x, z) \tag{4}
\end{equation*}
$$

Here, $z_{2}$ and $z_{1}$ are the upper and lower limits of integration, $\Delta z$ is the step size, and $f^{(4)}(x, z)$ is the fourth derivative of the integrand with respect to $z$, the integration variable. In the present case the step size was taken as 0.011 , the range of integration from 0 to 55 , corresponding to 5000 integration points. For this size grid, the truncation error given in Eq. (4) is negligible compared with computer round-off error.

TABLE I
Comparison of Approximate and Exact Calculations for $V(0.5, x)$

| $x$ | $U(0.5, x)^{a}$ | $U(0.5,-x)^{b}$ | $V(0.5, x)$ |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  |  | Exact $^{c}$ | This work $^{d}$ |
| 2.5 | $0.74258(-1)^{d}$ | $1.18833(1)$ | 3.80649 | 3.80622 |
| 2.6 | $0.63320(-1)$ | $1.35205(1)$ | 4.32412 | 4.32388 |
| 2.7 | $0.53770(-1)$ | $1.54548(1)$ | 4.93675 | 4.93655 |
| 2.8 | $0.45470(-1)$ | $1.77493(1)$ | 5.66444 | 4.66426 |
| 2.9 | $0.38288(1)$ | $2.04820(1)$ | 6.53197 | 6.53181 |
| 3.0 | $0.32104(-1)$ | $2.37497(1)$ | 7.57012 | 7.56998 |
| 3.1 | $0.26803(-1)$ | $2.76730(1)$ | 8.81724 | 8.81712 |
| 3.2 | $0.22281(-1)$ | $3.24027(1)$ | $1.03213(1)$ | $1.03212(1)$ |
| 3.3 | $0.18441(-1)$ | $3.81279(1)$ | $1.21425(1)$ | $1.21424(1)$ |
| 3.4 | $0.15196(-1)$ | $4.50871(1)$ | $1.43566(1)$ | $1.43565(1)$ |
| 3.5 | $0.12468(-1)$ | $5.35814(1)$ | $1.70594(1)$ | $1.70594(1)$ |
| 3.6 | $0.10184(-1)$ | $6.39931(1)$ | $2.03729(1)$ | $2.03729(1)$ |
| 3.7 | $0.82810(-2)$ | $7.68095(1)$ | $2.44519(1)$ | $2.44518(1)$ |
| 3.8 | $0.67038(-2)$ | $9.26532(1)$ | $2.94948(1)$ | $2.94946(1)$ |
| 3.9 | $0.54027(-2)$ | $1.12324(2)$ | $3.57556(1)$ | $3.57556(1)$ |
| 4.0 | $0.43344(-2)$ | $1.36853(2)$ | $4.35630(1)$ | $4.35629(1)$ |

${ }^{a}$ Ref. [1].
${ }^{b}$ Eq. (3).
${ }^{c}$ From the Hermite polynomials, Eq. (5).
${ }^{d}$ Eq. (1).
" Numbers in parcntheses are powers of ten.

Table I gives an indication of the accuracy of these calculations. Here we show values of $V(a, x)$ via Eq. (1) for $\mathbf{a}=0.5$ and $\mathbf{x}$ in the range of interest discussed in [1], $2.5 \leqslant x \leqslant 4.0$. This value of a was chosen because exact results may be obtained for $V\left(n+\frac{1}{2}, x\right)$ ( $n$ integral) from the Hermite polynomials [5]:

$$
\begin{align*}
V(n+1 / 2, x) & =(2 / \pi)^{1 / 2} \exp \left(x^{2} / 4\right) H e_{n}^{*}(x)  \tag{5}\\
H e_{n}^{*}(x) & =\exp \left(-x^{2} / 2\right) \frac{d^{n}}{d x^{n}} \exp \left(x^{2} / 2\right)
\end{align*}
$$

The results of [1] were used for $U(a, x)$ in Eq. (1), while Eq. (3) provided the values of $U(a,-x)$. Errors in these results are due almost entirely to those generated for $U(a, x)$ given in [1] to which the reader is referred.

In conclusion, the results shown in this note and in [1] demonstrate a method of calculating the parabolic cylinder functions which is simpler than the usual power series methods and is applicable in ranges of argument where these other methods do not converge.

## References

1. W. P. Latham and R. W. Redding, J. Computational Phys. 16 (66) (1974).
2. M. Abramowitz and I. Stegun, "Handbook of Mathematical Functions," National Bureau of Standards Applied Mathematics Series 55, Washington, D.C., 1964, p. 687. Eq. (19.4.2).
3. I. S. Gradshteyn and I. M. Ryzhik, "Tables of Integrals, Series, and Products," Academic Press, New York, 1965, p. 337. Eq. 3.462.1.
4. P. A. Stark, "Introduction to Numerical Methods," MacMillan Co., New York, 1970, pp. 192-212.
5. Ref. 2, p. 691. Eq. (19.13.2).

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